GAMMA RESPONSES FOR A NEUTRON PULSING “ANDA” EXPERIMENT

AS COMPUTED BY THE BATEMAN EQUATIONS, ORIGEN-S, AND DECAYCALC

B. Ludewigt, K. Alfonso, D. Chivers, R. Crabbs, B. Goldblum, J. Lorenzo

Dec 16, 2009

1. COMPUTATIONAL METHODS

This active interrogation project began with code that analytically solved the Bateman equations to track the decays of fission products after neutron irradiation. Our goal now is to benchmark the predictions of the analytical model with those from other simulations.

ORIGEN-S is the standard tool for tracking the growth and decay of radioactive nuclides. The tool also now features an ability to output the gamma spectra produced from the decay of nuclides in a sample. This allows us to directly use ORIGEN-S for benchmarking of the analytical approach.

Another tool available to us is the decayCalc Python toolchain. This code has no ability to compute growth and decay of nuclides, so it is necessary to feed it a time-dependent description of the sample composition. From there, decayCalc searches TORI databases to find the type, energy, and intensity of decays released. It has the additional ability to transport these particle spectra through MCNPX for detector simulations.

For this first round of simulations, a few simplifications have been made. First, we have neglected the length of irradiation time, treating each activation step as a delta pulse of neutrons. This is reasonable, as the signals of interest to us are produced by nuclides with half-lives longer than a second. (The pulse lengths are likely to be 200ms, with a 20ms cool-off before gamma counting begins.)

Secondly, we have not yet implemented neutron transport, for computing physical reaction rates. We have not fully laid out the geometry of an experimental device, so accounting for the neutron transport is not productive. Similarly, we have not accounted for the transport of the gamma rays produced by spontaneous decays in the irradiated sample.

Thirdly, all fissions are assumed to be by thermal neutrons incident on U-235. Preliminary neutron profiles show that the thermal to fast fission ratio is on the order of 100.

The ORIGEN-S simulations modeled the neutron pulsing in the following way:

1. A flux of neutrons incident on a highly-enriched target produces 1000 thermal U-235 fissions. The resulting fission fragments (gathered from the England and Rider distributions) are fed into ORIGEN-S for a 10-second decay.
2. The nuclides leftover at the end of the 10-second counting period are then combined with a fresh set of fission fragments, and recycled into ORIGEN-S for another 10-second decay case.

A total of 10 such cycles were performed, each of which added the products of 1000 fissions to the mix. Final composition data was recorded during the 10^{th} counting period (10s long). In addition, ORIGEN-S output the gamma spectrum emitted during this time.

2. DETAILS OF THE SIMULATIONS

The analytical model produced time-dependent gamma responses for 10 key energy bins. These bins are centered at 1506keV, 1512keV, 1644keV, 1710keV, 1836keV, 1905keV, 2079keV, 2238keV, 2349keV, and 2820keV, and each is 3keV wide, reflecting the energy resolution of a typical HPGe detector.

Both decayCalc and ORIGEN-S used these exact energy bin boundaries.

For the following sets of figures, the gamma response is given in gammas per 50ms. (These are the original units used for plots of analytical results.) Note, however, that the decayCalc simulation used a coarser time binning of 0.25s, so the output gamma responses were uniformly divided by a factor of 5 for direct comparison.

Note that the decayCalc tool only has two modes--"steady state" and "batch decay". In the "steady state" mode, compositions are held constant during a time bin. In the "batch decay" mode, all radioactive nuclides simply decay away, which neglects the behavior of decay chains during a time step. For these simulations, we used the "batch decay" mode.

Still, the decayCalc results tend to be much closer to the original analytical results. While the ORIGEN-S simulation used the exact time and energy bin settings, it used a different set of decay libraries for its computations. (The decayCalc and analytical calculations used the most recent TORI databases, which are significantly newer than the libraries used by ORIGEN.)

3. RESULTS

For the gamma spectra produced by ORIGEN-S, there are only two categories of plot: those with good agreement with the analytical model and those that have no agreement whatsoever.

GOOD AGREEMENT
1512keV
1905keV
2238keV
2820keV

DECENT AGREEMENT
1506keV (t ~ 0 value from ORIGEN is too low)
1644keV (A factor of ~2 off, but similar shape)
2079keV (t ~ 0 value from ORIGEN is too low)
2349keV (A factor of ~2 off, but similar shape)

TOTAL DISAGREEMENT
1710keV (Completely wrong shape)
1836keV (Wrong shape and wrong order of magnitude)

The 1506keV and 2079keV plots actually match the analytic model's pretty well except for the very early times. We expect the ORIGEN library simply is missing data on a short-lived nuclide.

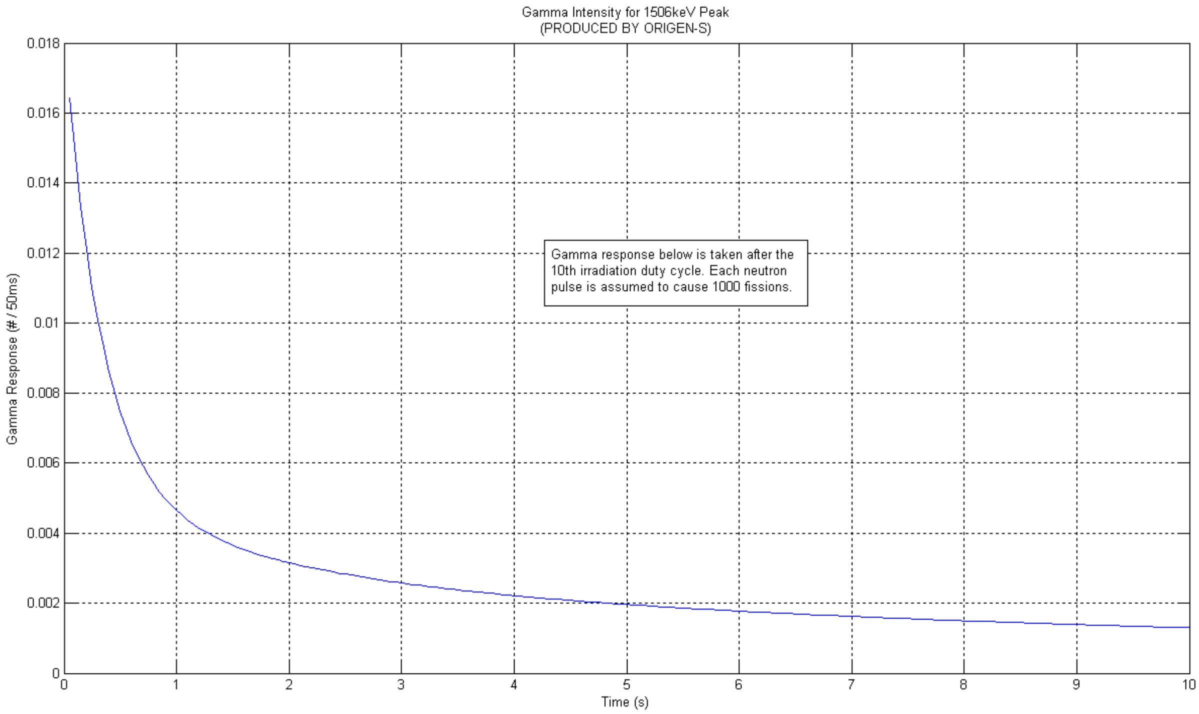
Note that ORIGEN-S uses its own decay library to compute the gamma emissions in a sample. Both decayCalc and the analytic model use the TORI database.

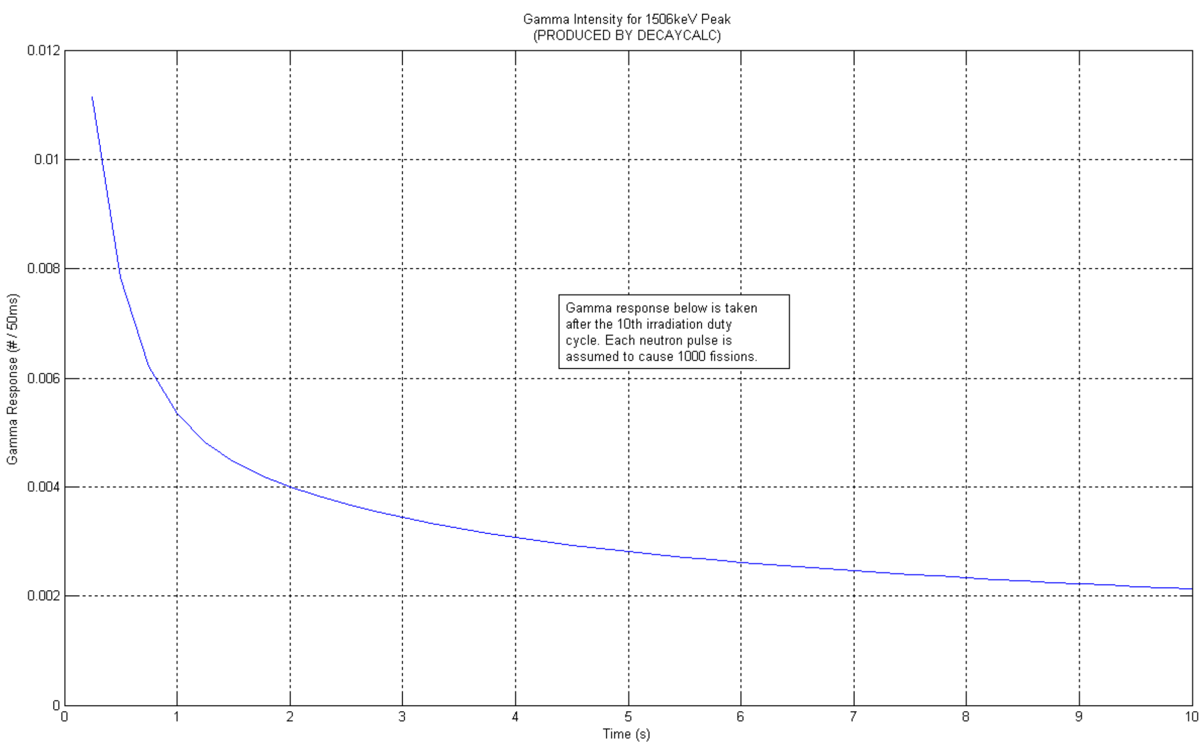
The good news is that most of the decayCalc figures show good agreement with those produced by the analytic approach. In general, we noticed the intensity of the gammas is a little higher for the analytic model, at least for earlier times. Sometimes, the decayCalc responses have greater magnitudes, but only after 9s or so into the counting period.

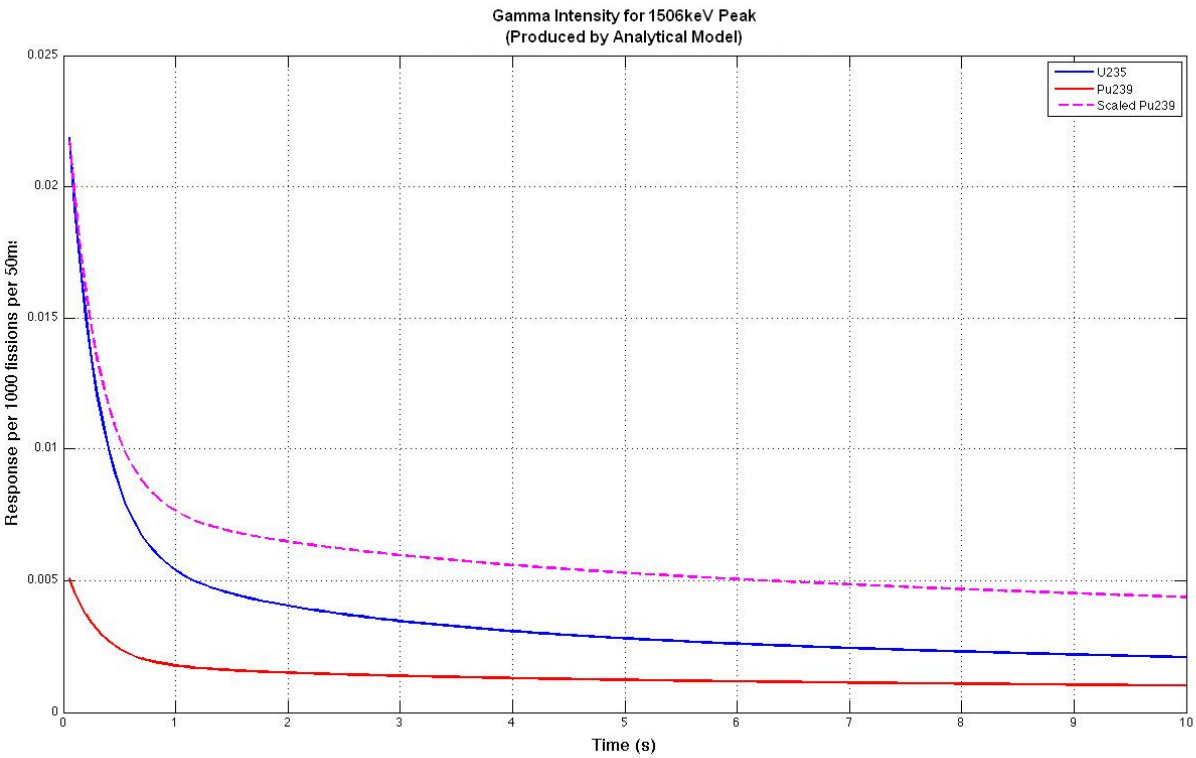
In both cases, the differences between models is less than 25% (with one exception at 1506keV). Generally, the differences are even less, perhaps on the order of 10%.

For the 1506keV energy bin, the decayCalc results were a factor < 2 lower than those from the analytical Bateman model. Also, the decayCalc response did not drop off as quickly.

Gamma Responses for 1506keV

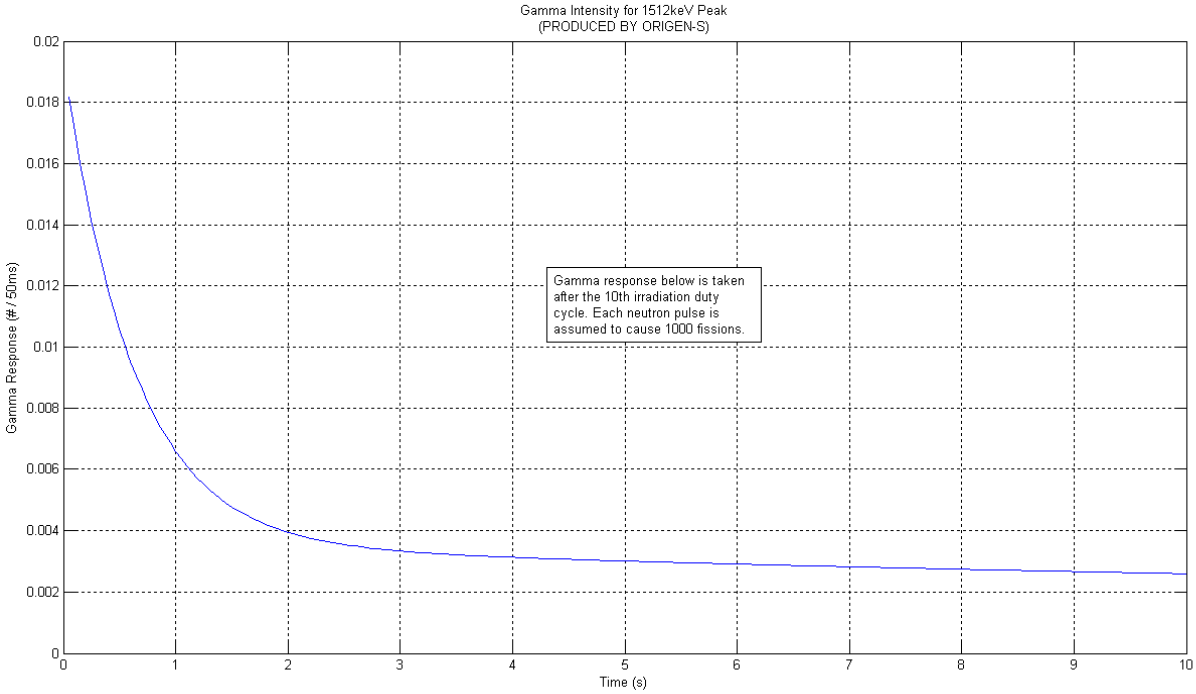


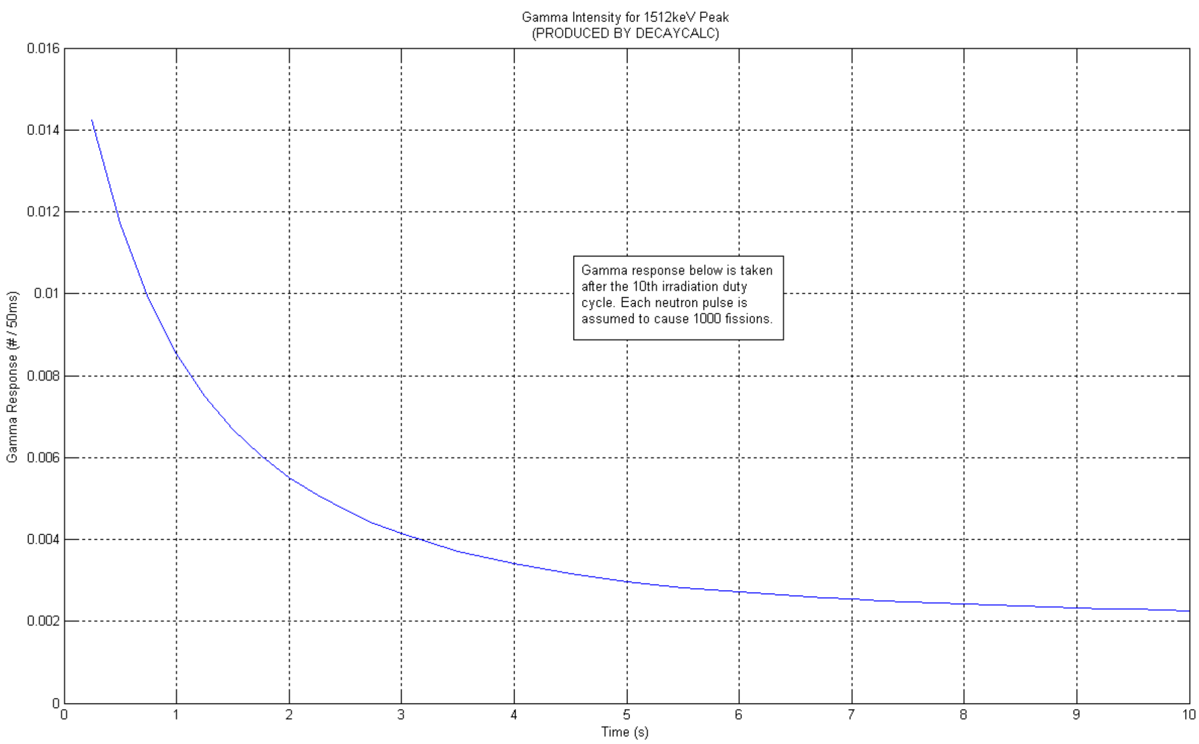


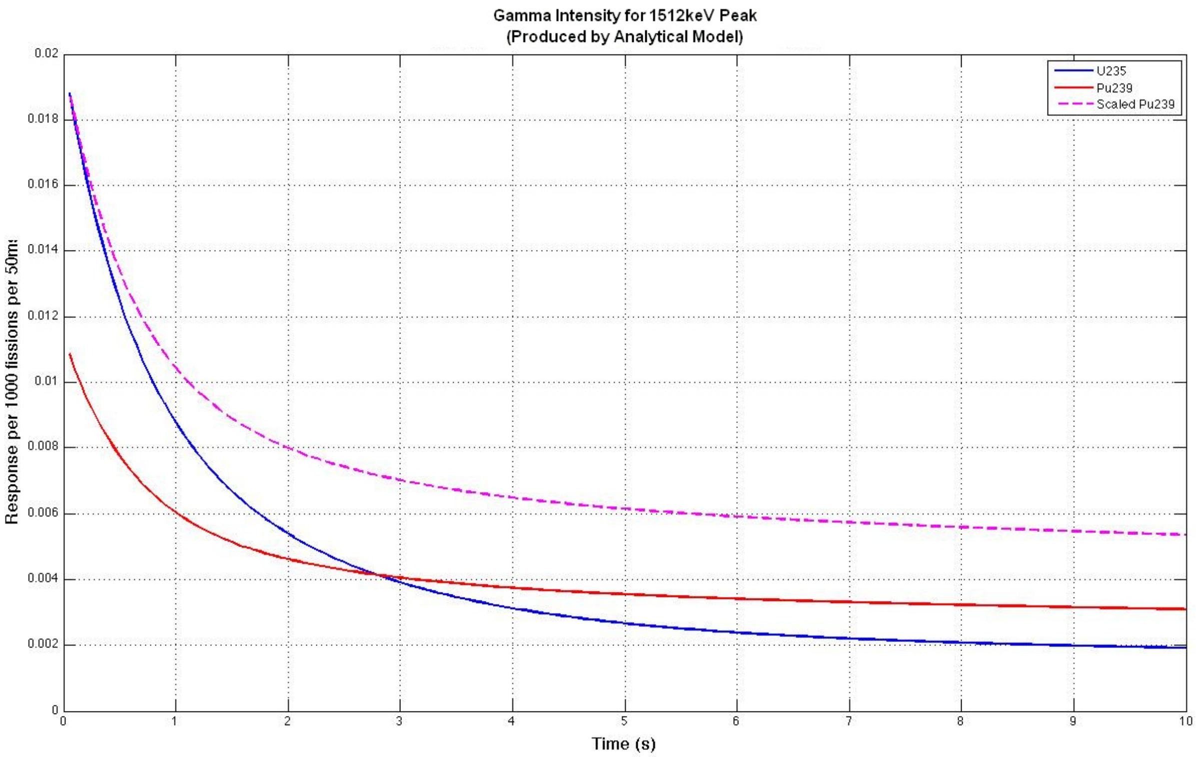


Gamma Intensity for 1506keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7
8
9
10

Gamma Responses for 1512keV

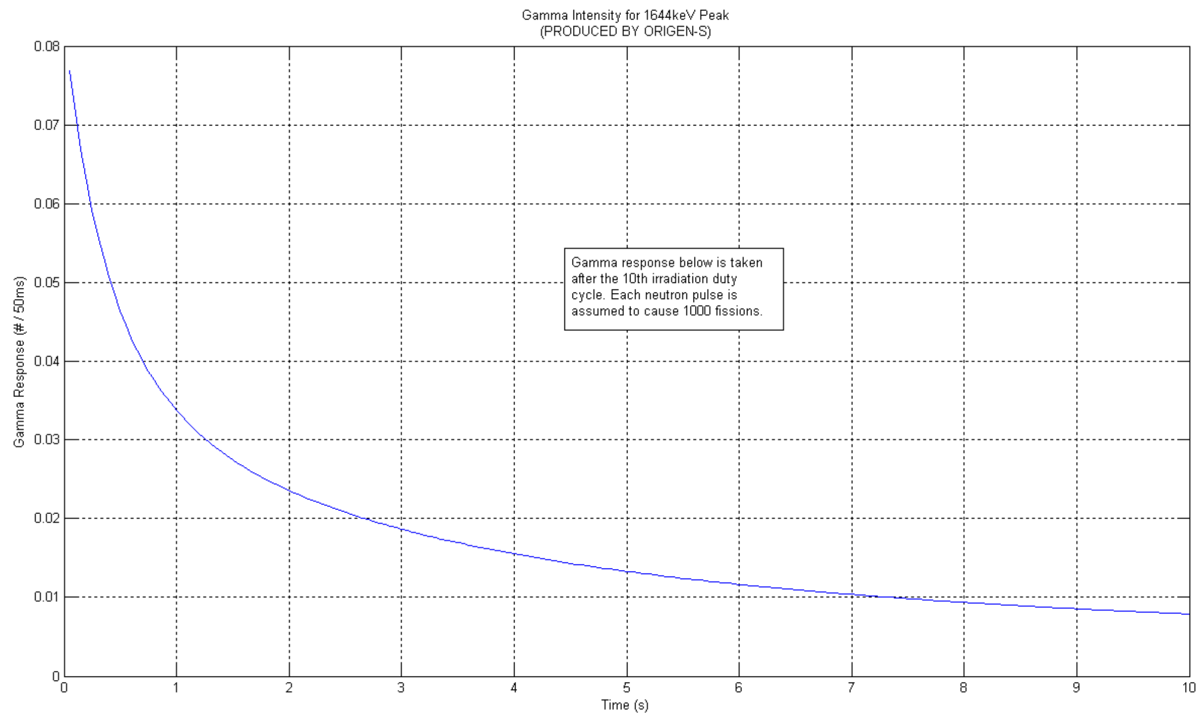


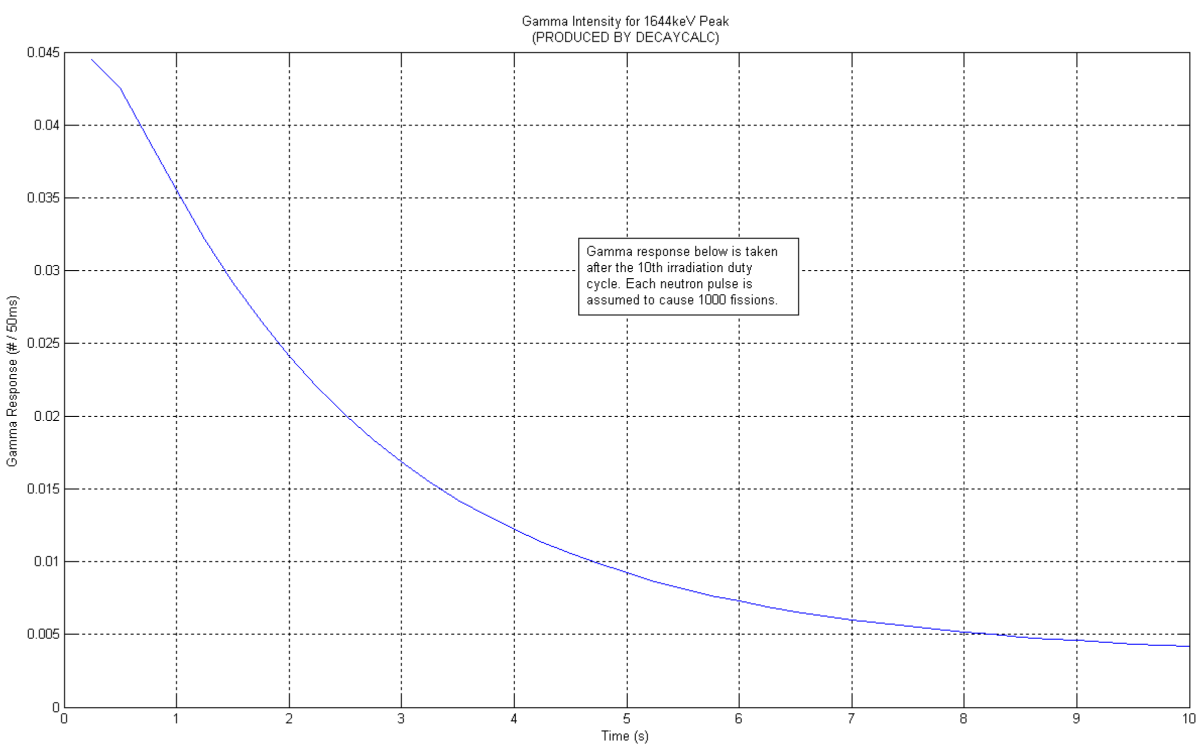


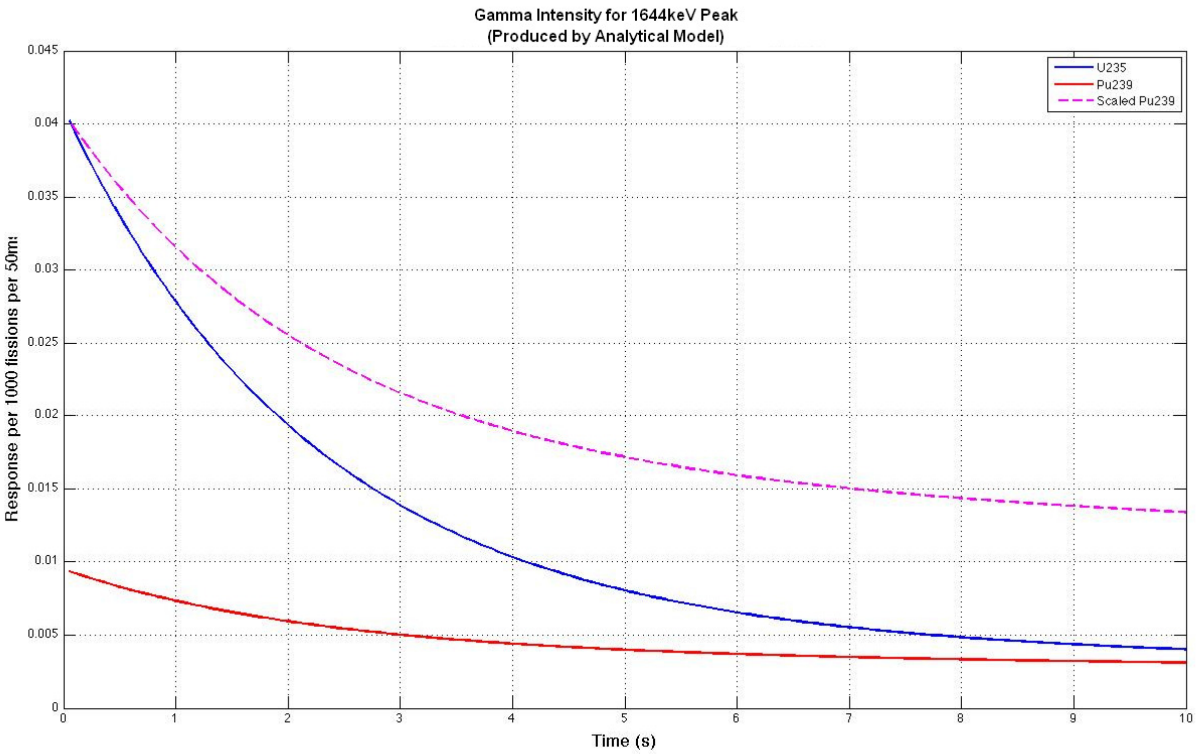


Gamma Intensity for 1512keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0
0.002
0.004
0.006
0.008
0.01
0.012
0.014
0.016
0.018
0.02
0
1
2
3
4
5
6
7
8
9
10

Gamma Responses for 1644keV

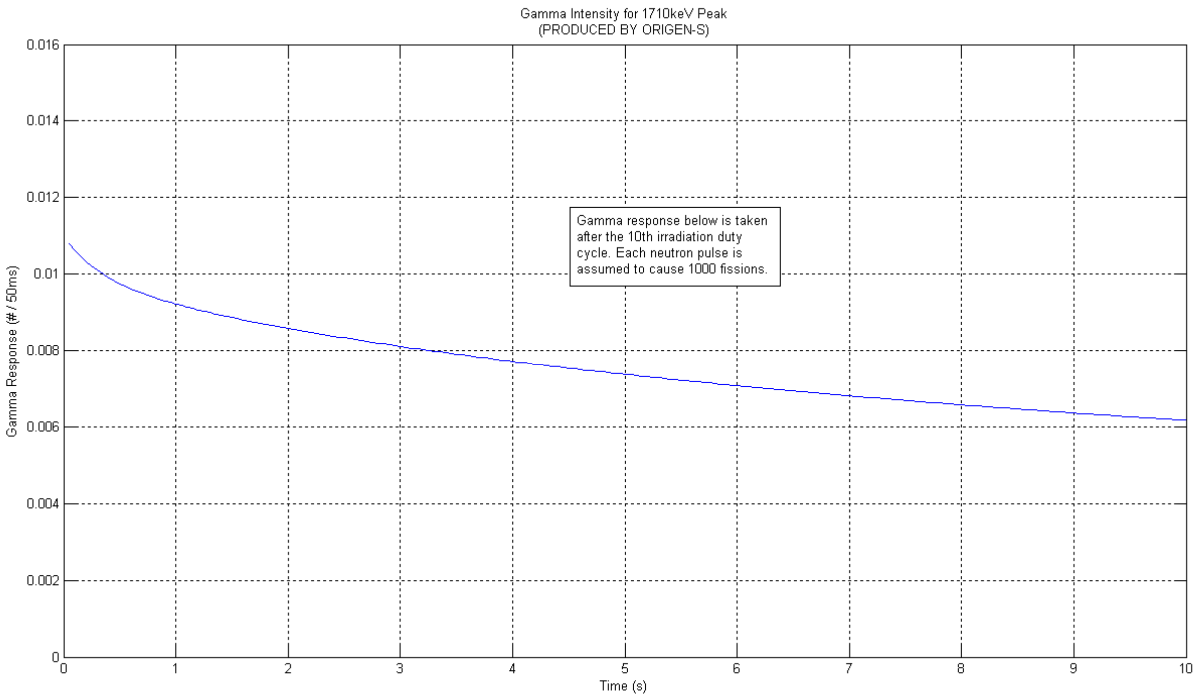


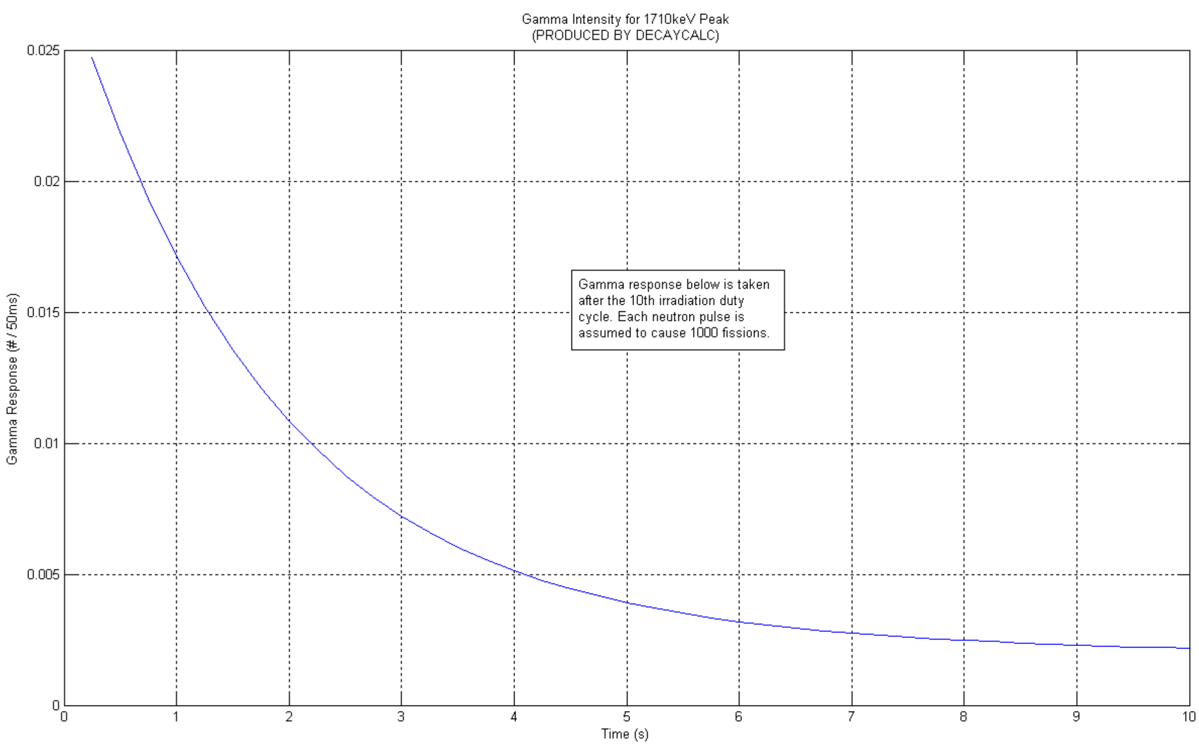


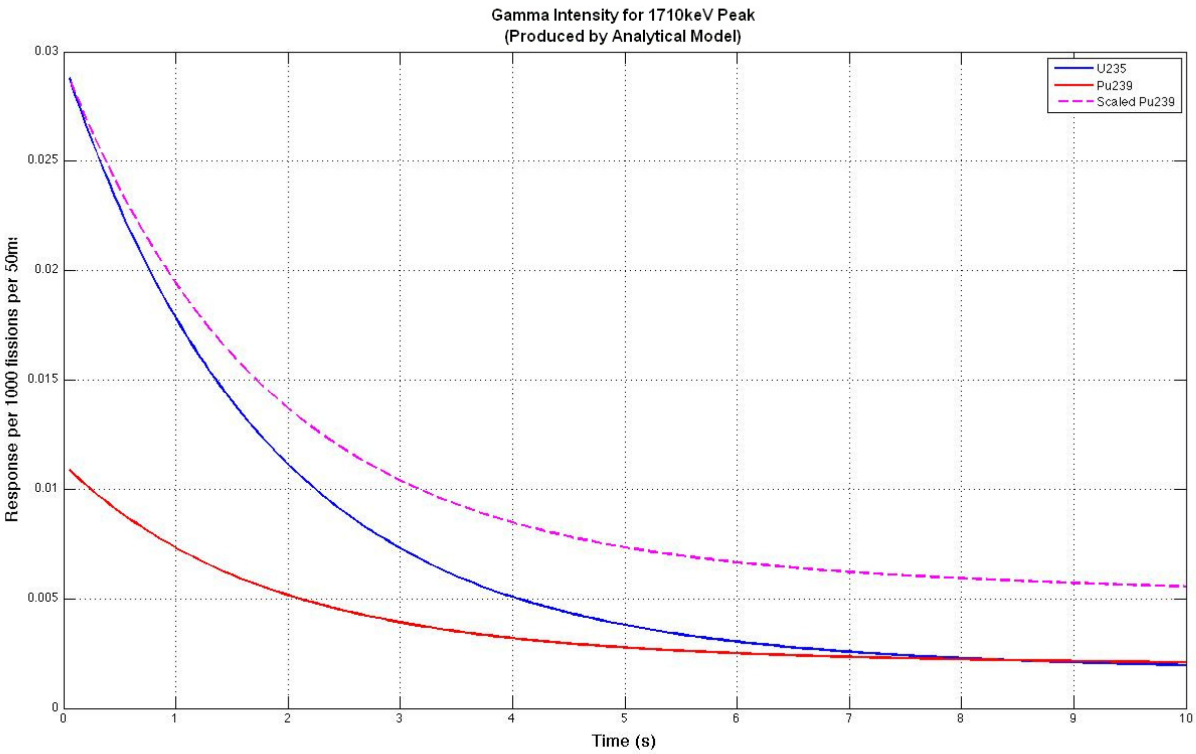


Gamma Intensity for 1644keV Peak
(Produced by Analytical Model)
Response per 1000 fissions per 50ms
Time (s)
U235
Pu239
Scaled Pu239
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7
8
9
10

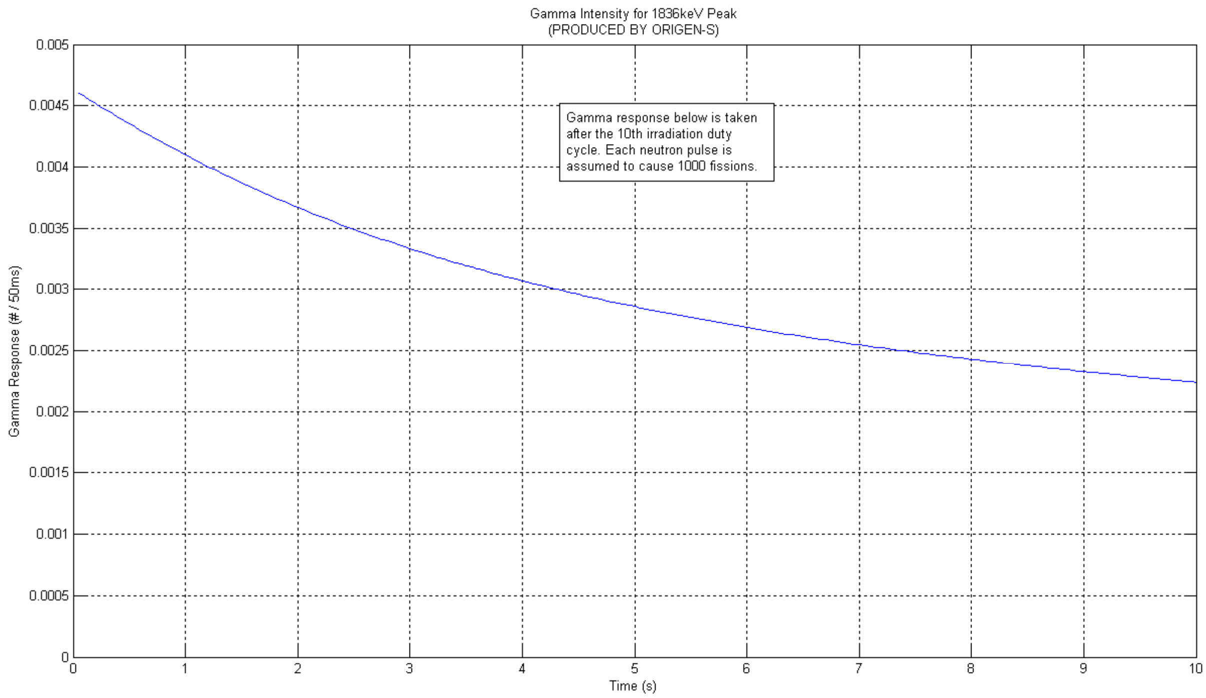
Gamma Responses for 1710keV

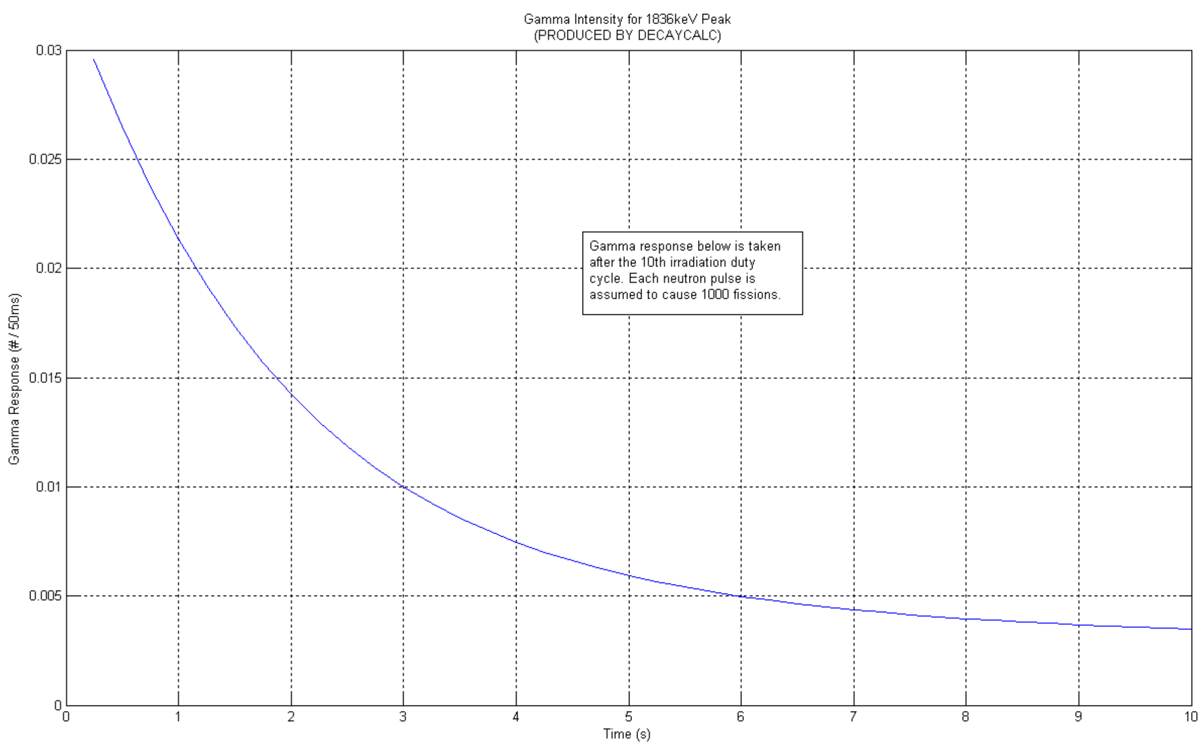


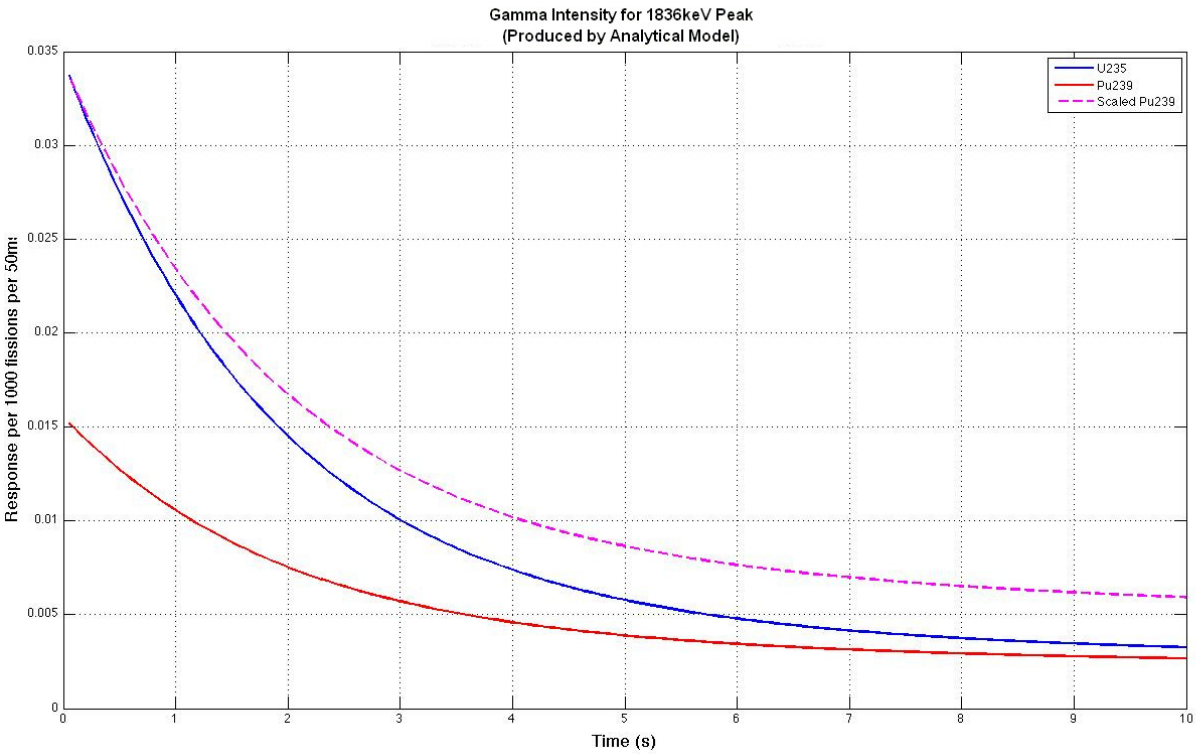



Gamma Intensity for 1710keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0
0.005
0.01
0.015
0.02
0.025
0.03
0
1
2
3
4
5
6
7
8
9
10

Gamma Responses for 1836keV

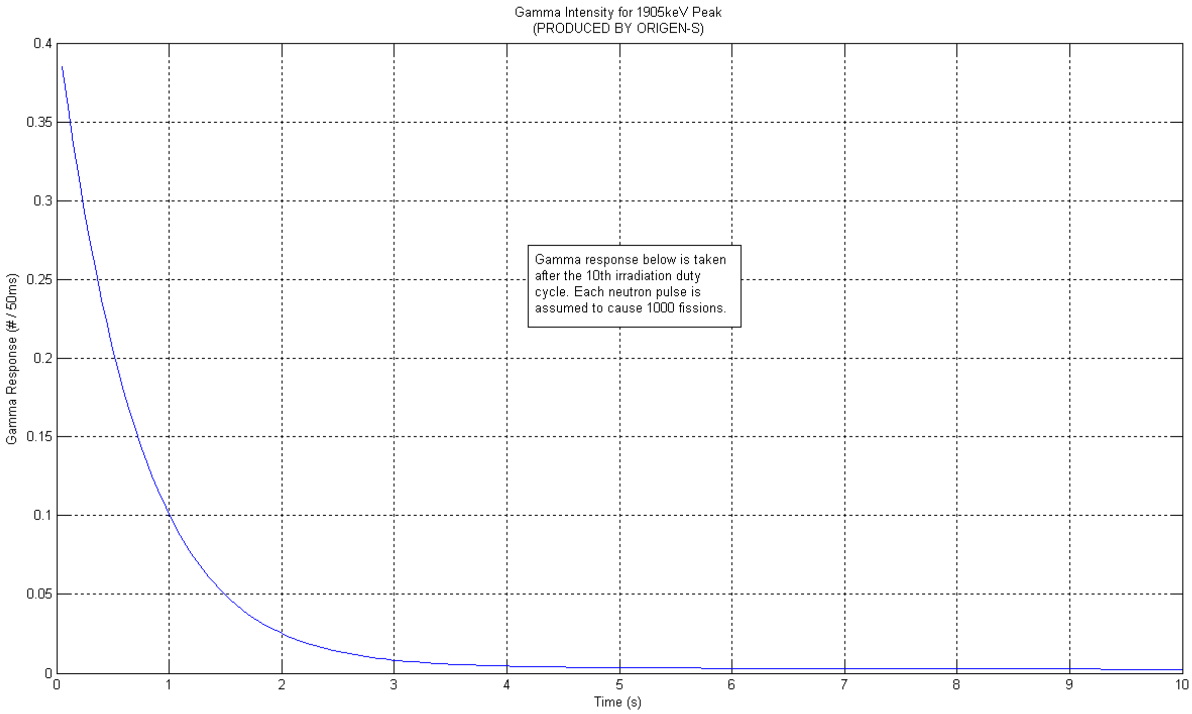


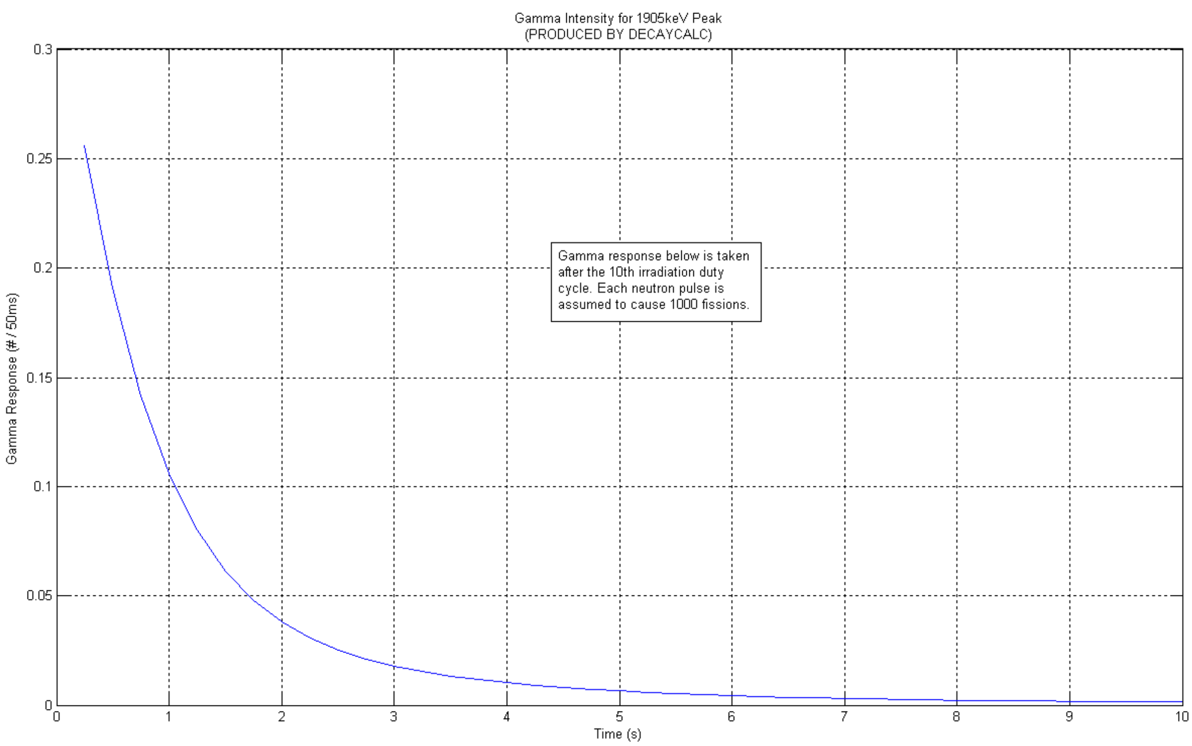


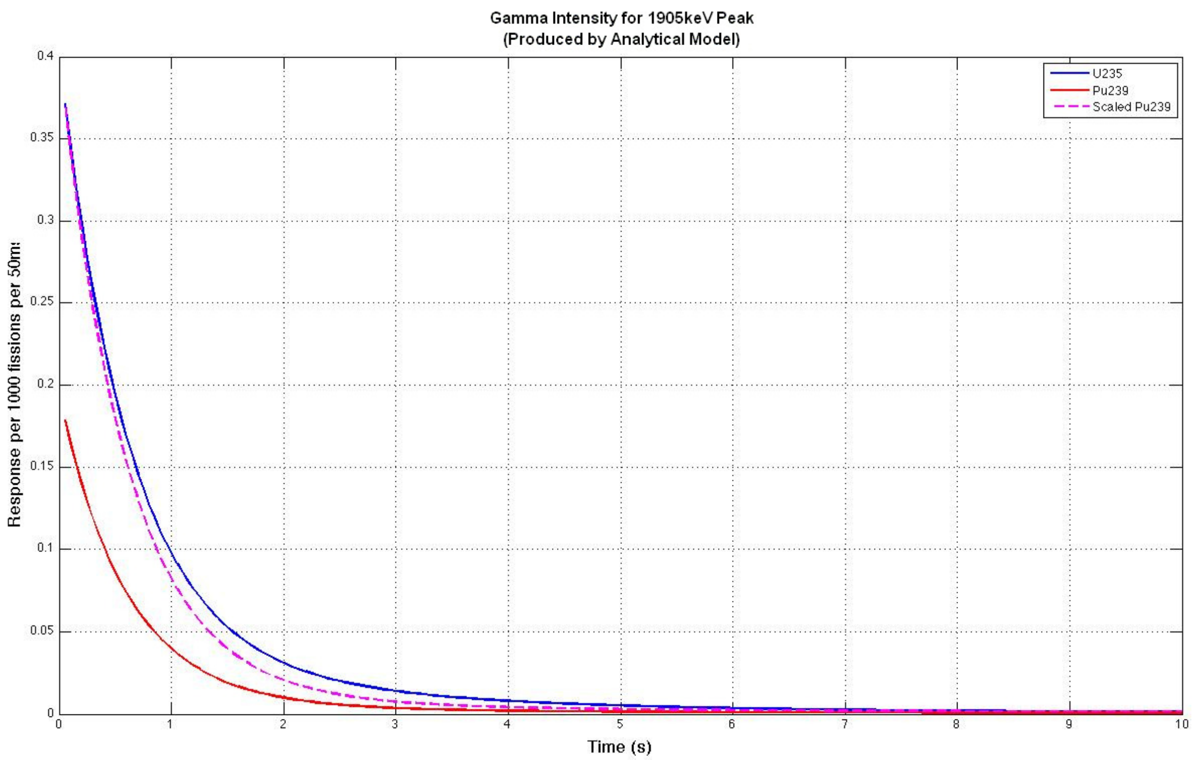


Gamma Intensity for 1836keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7
8
9
10

Gamma Responses for 1905keV

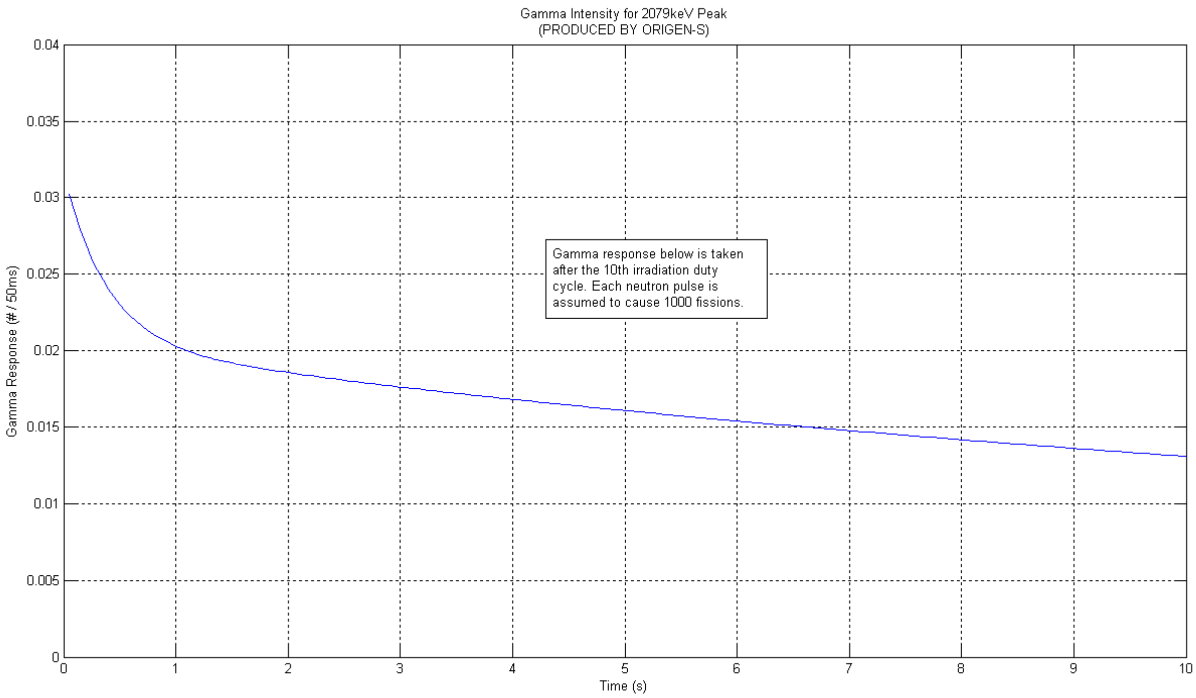


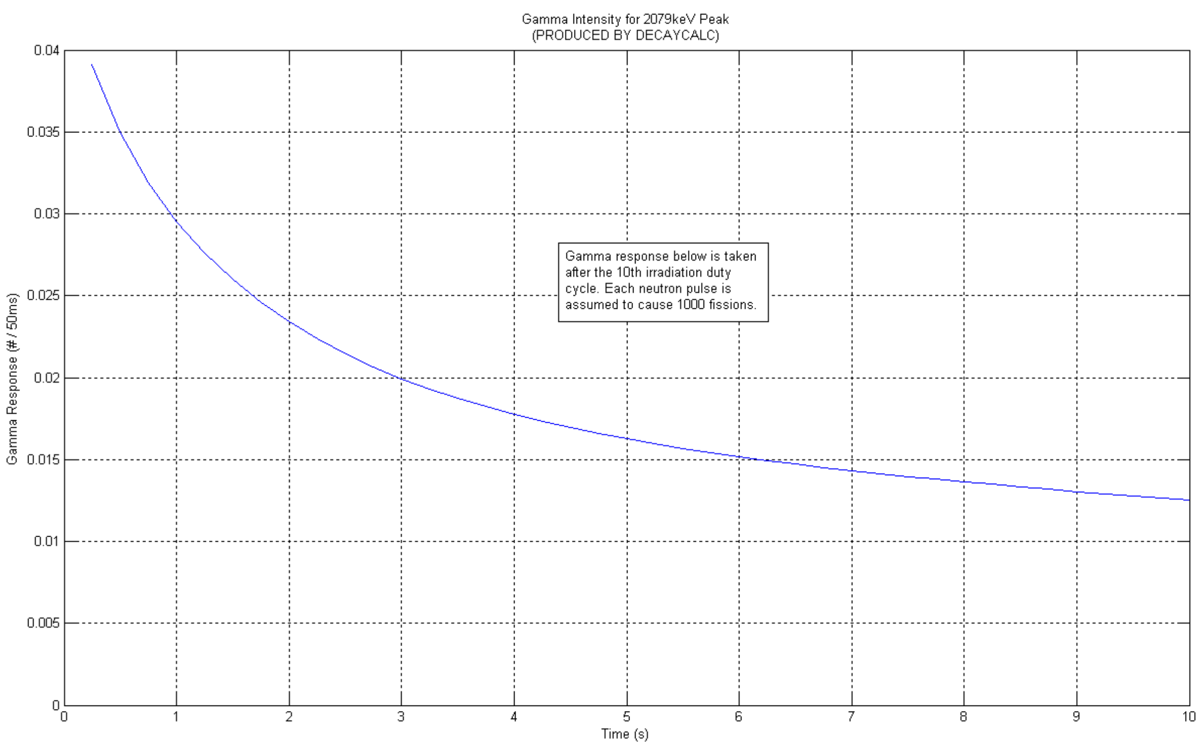


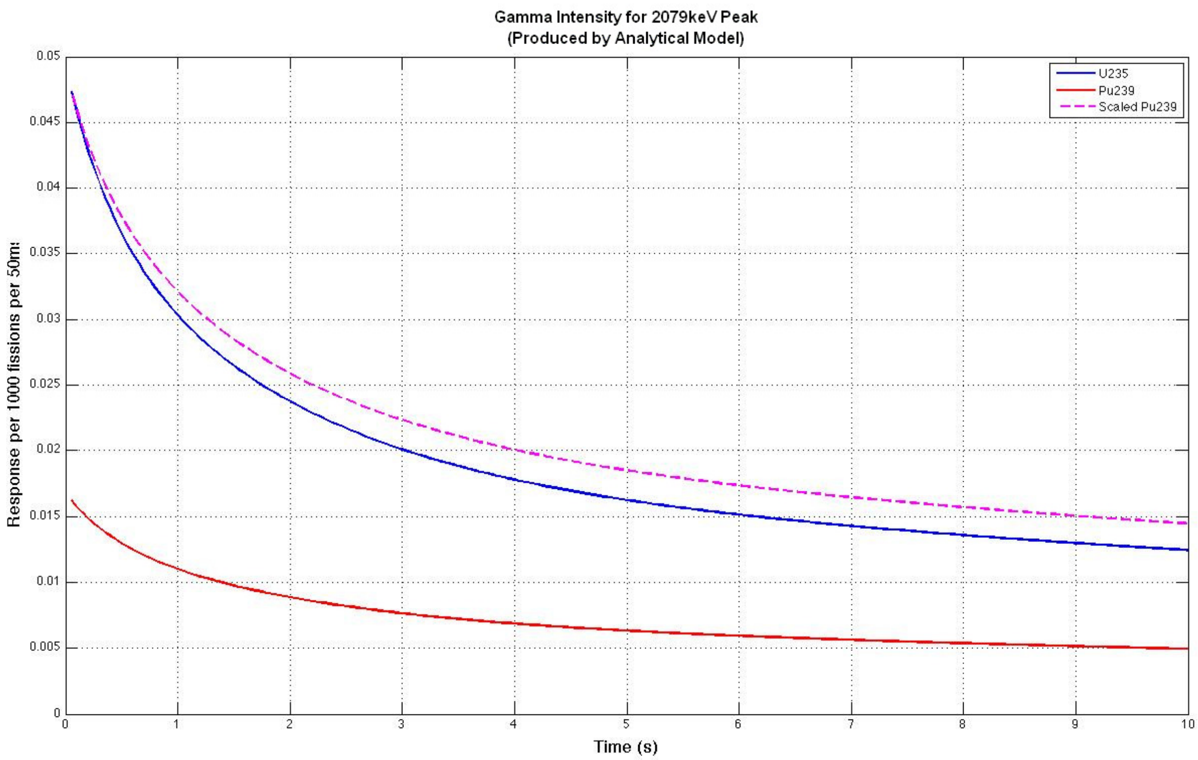


Gamma Intensity for 1905keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0
1
2
3
4
5
6
7
8
9
10
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05

Gamma Responses for 2079keV

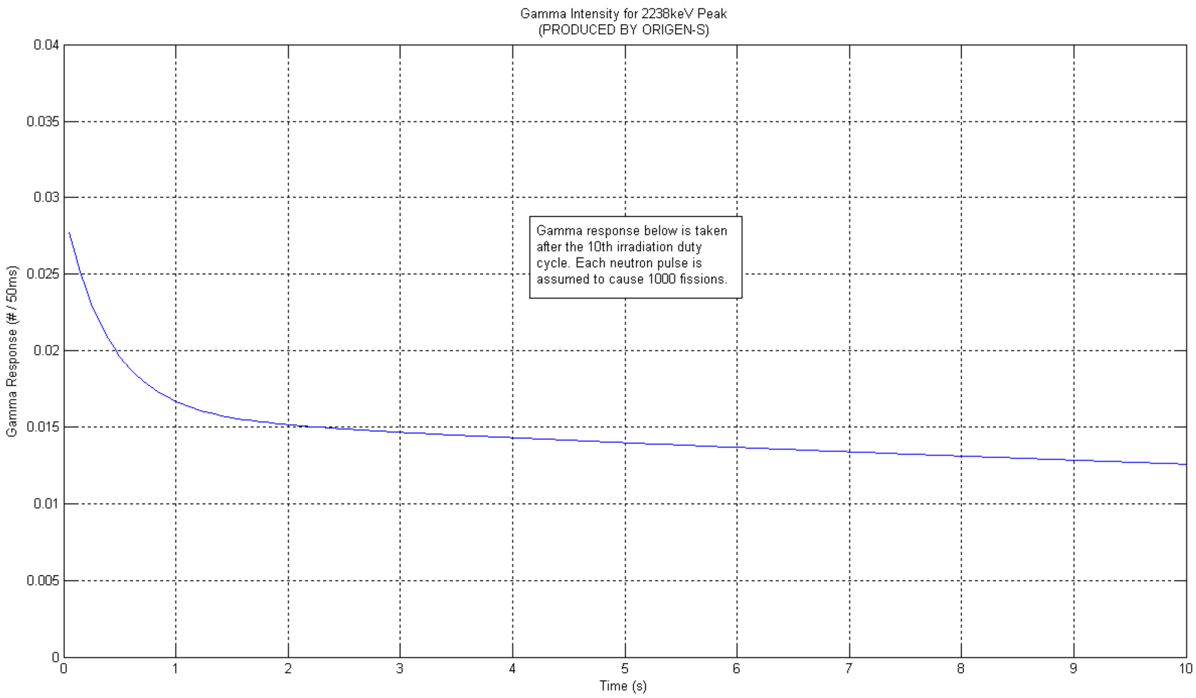


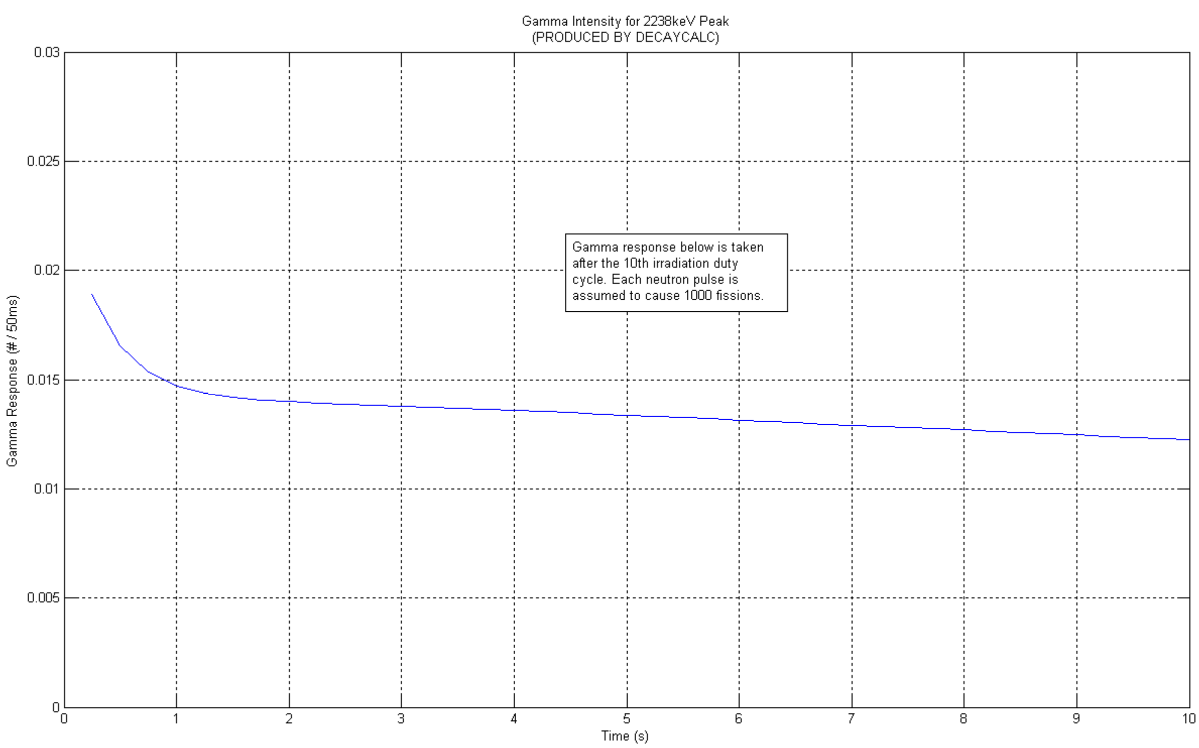


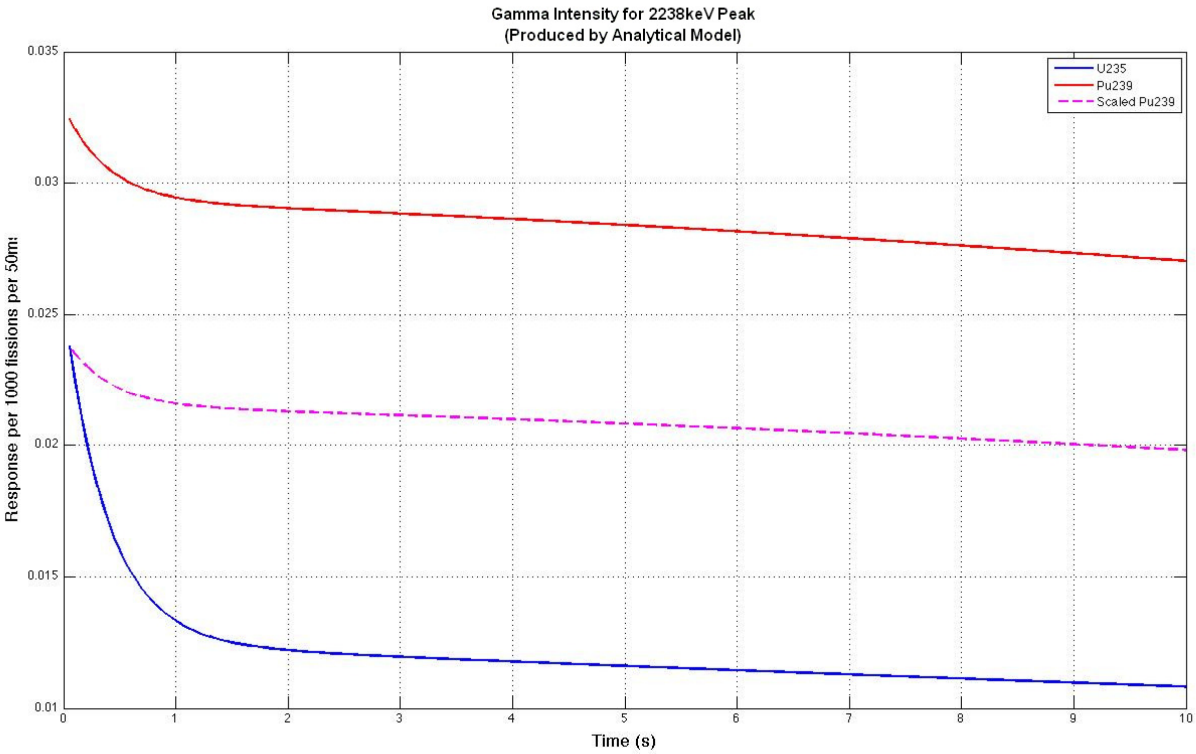


Gamma Intensity for 2079keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05
0
1
2
3
4
5
6
7
8
9
10

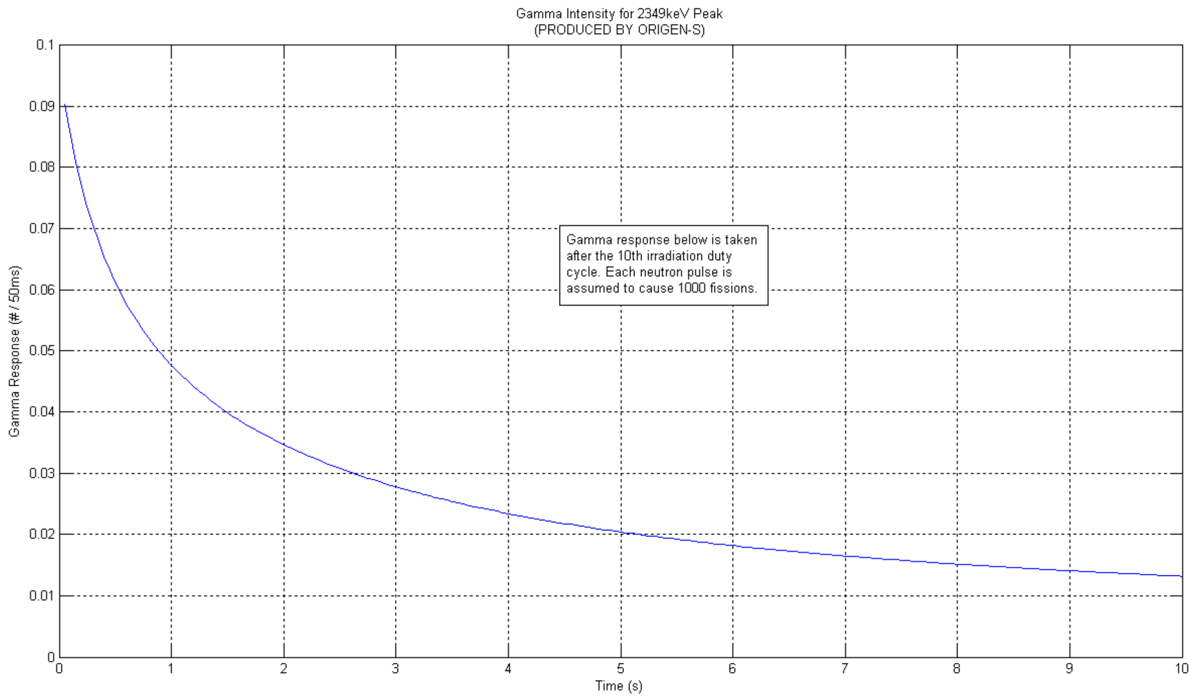
Gamma Responses for 2238keV

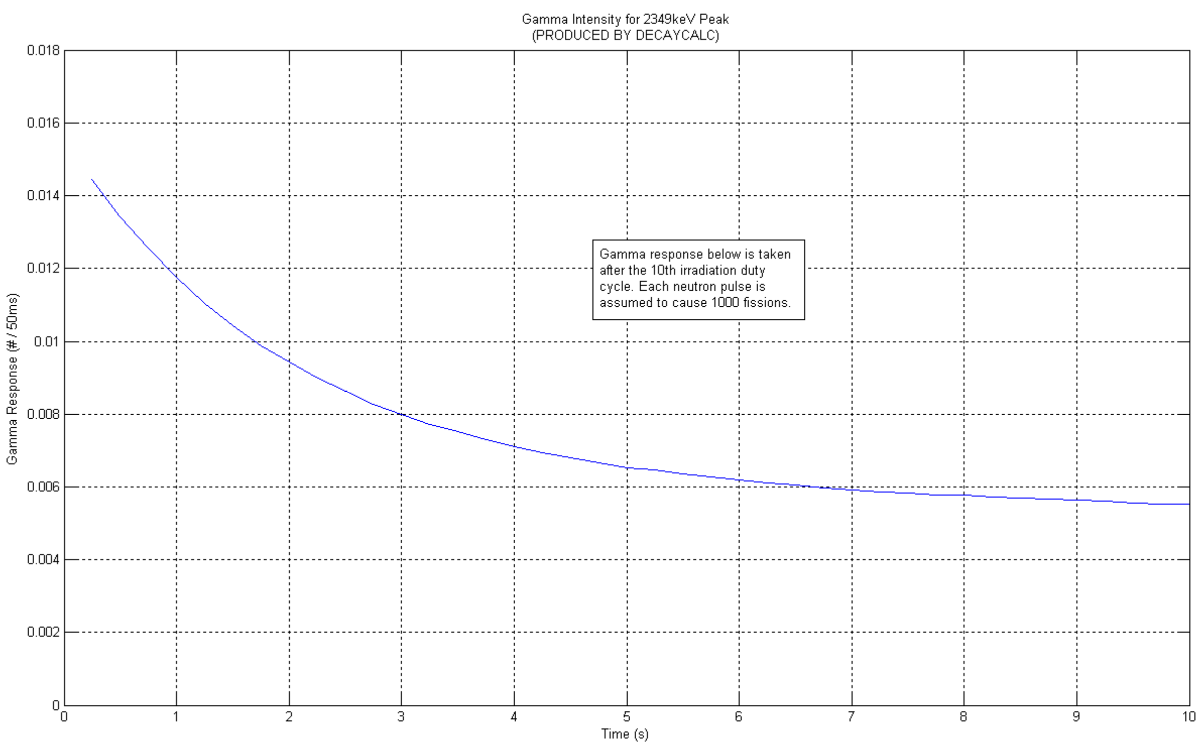


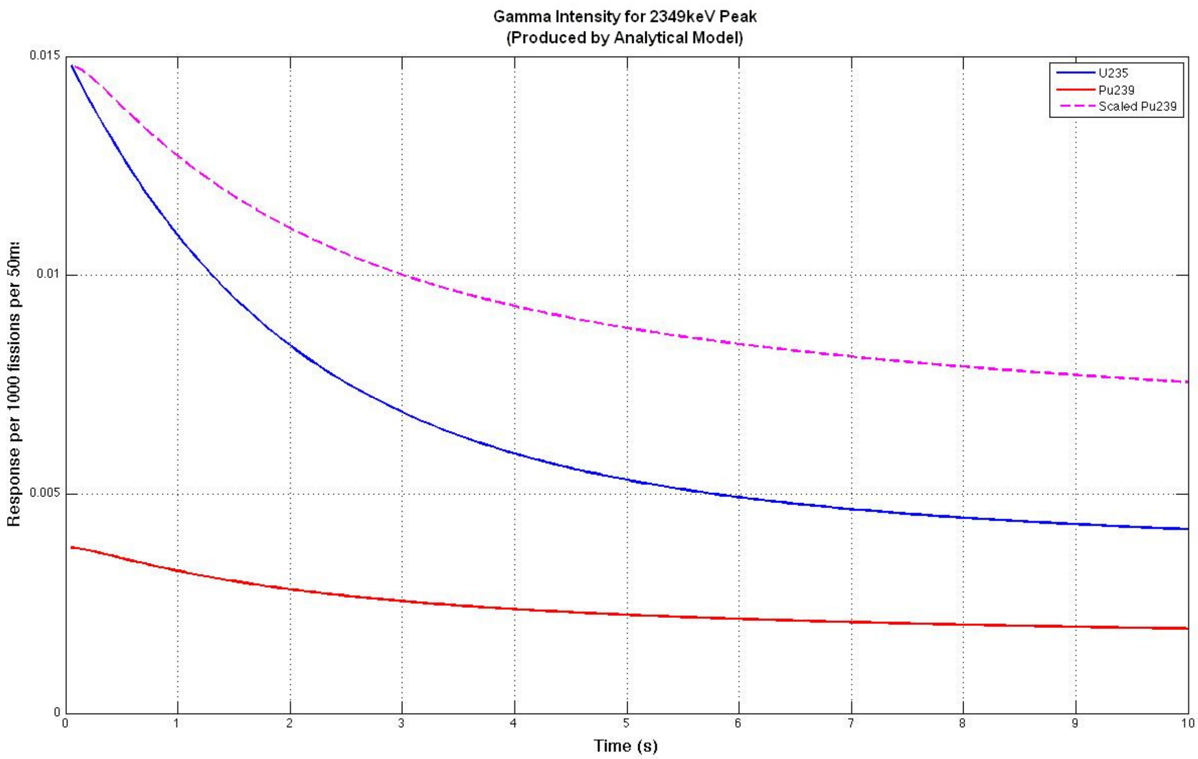



Gamma Intensity for 2238keV Peak
(Produced by Analytical Model)
Response per 1000 fissions per 50ms
Time (s)
U235
Pu239
Scaled Pu239
0.035
0.03
0.025
0.02
0.015
0.01
0
1
2
3
4
5
6
7
8
9
10

Gamma Responses for 2349keV

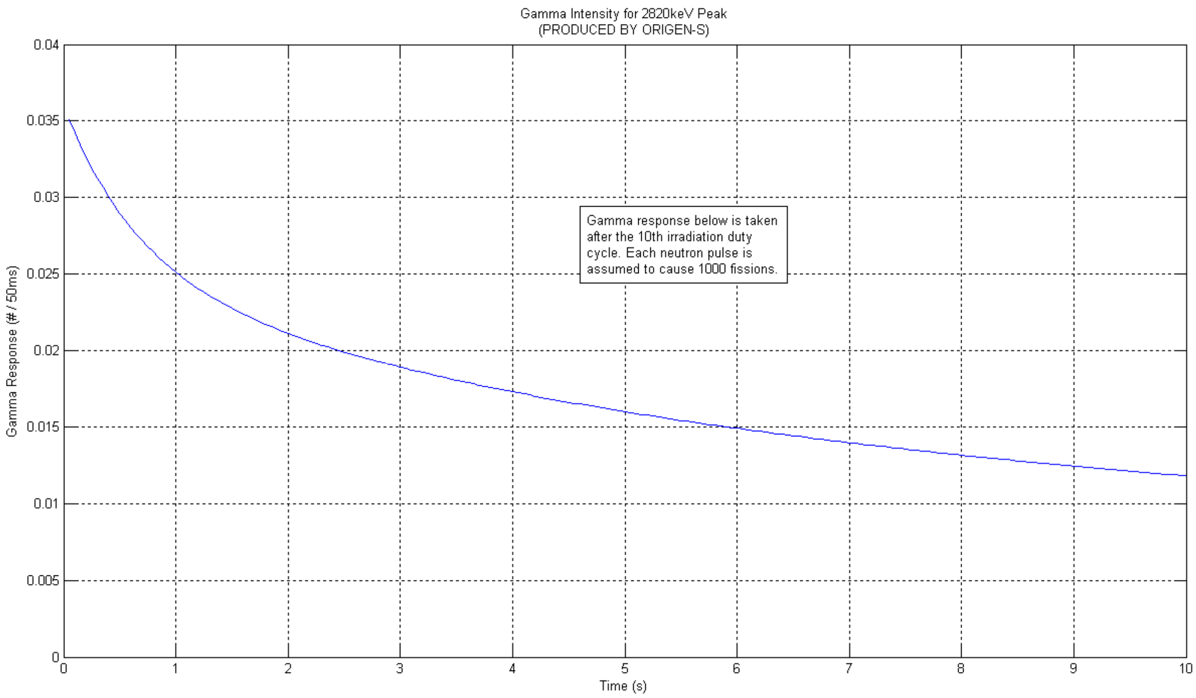


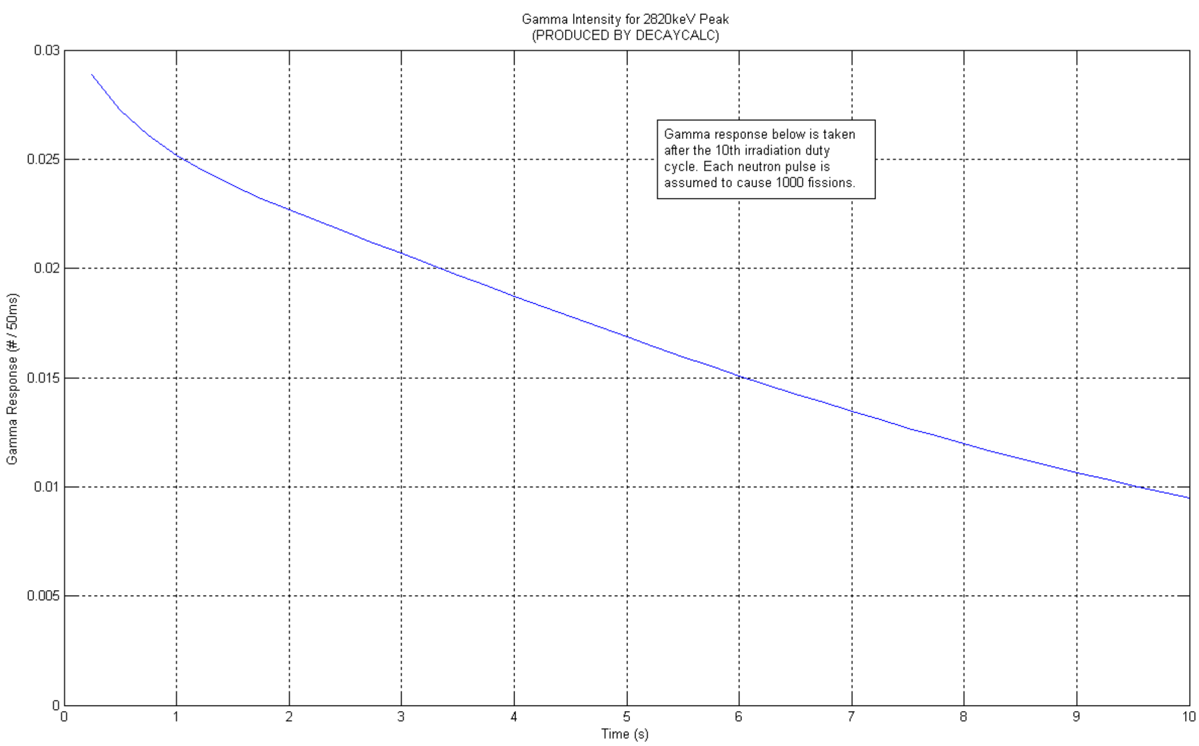


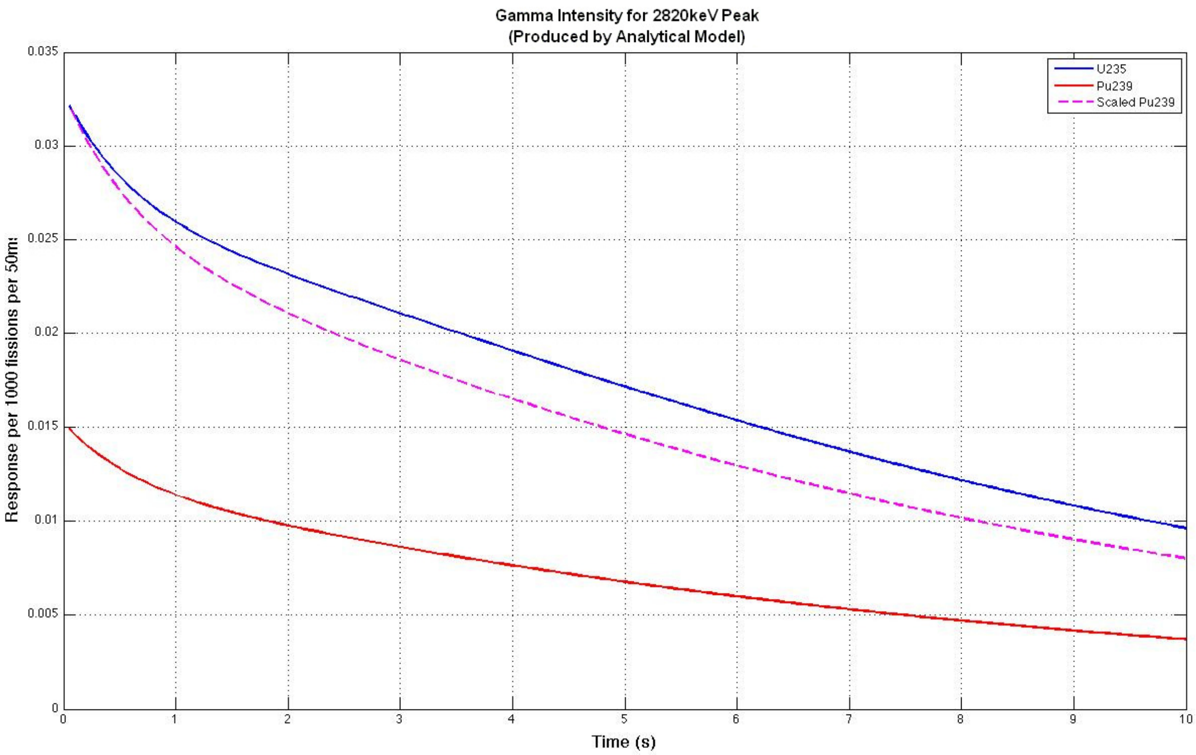


Gamma Intensity for 2349keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7
8
9
10
Time (s)

Gamma Responses for 2820keV






Gamma Intensity for 2820keV Peak
(Produced by Analytical Model)
U235
Pu239
Scaled Pu239
Response per 1000 fissions per 50ms
Time (s)
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0
1
2
3
4
5
6
7
8
9
10